

It is one of the most important needs to develop renewable, scalable and multifunctional methods for the *fabrication of 3D carbon architectures*. Even though a lot of methods have been developed to create porous and mechanically stable 3D scaffolds, the fabrication and control over the synthesis of such architectures still remain a challenge. Here, we used *Magnetospirillum magneticum*¹ (AMB-1) bacteria as a bio-template to *fabricate light-weight 3D solid structure of carbon nanotubes (CNT)* with interconnected porosity². The resulting porous scaffold showed good mechanical stability and large surface area because of the excellent pore interconnection and high porosity. *Steered molecular dynamics* simulations were used to quantify the interactions between nanotubes and AMB-1 via the cell surface protein MSP-1 and flagellin. The 3D CNT-AMB1 nanocomposite scaffold is further demonstrated as a potential *substrate for electrodes in supercapacitor applications*.

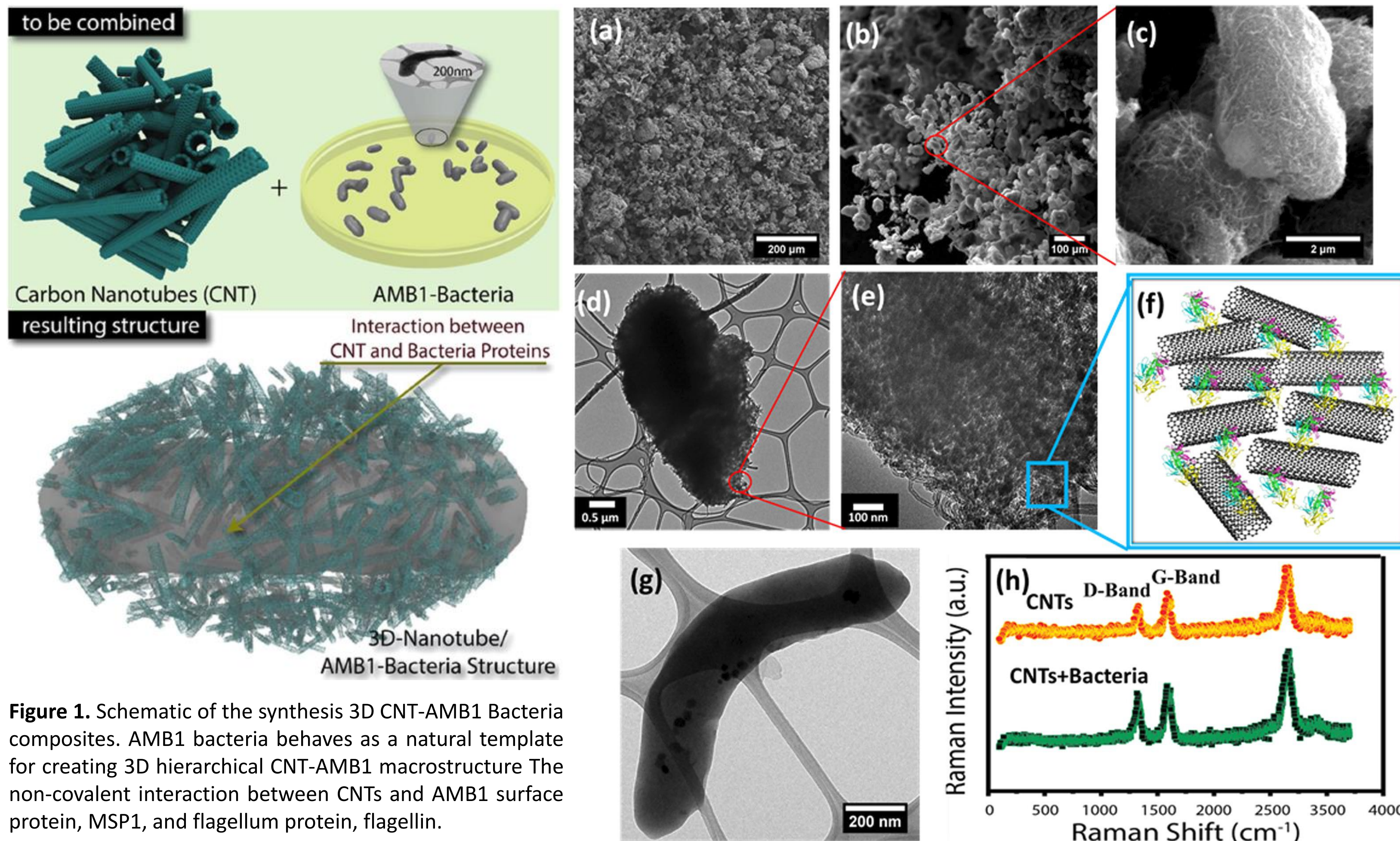


Figure 2. Microscopic and spectroscopic characterization of 3D nanotube/bacteria structure. (a–c) SEM images of CNT-bacteria structure shows that AMB1 bacteria acts as template for CNTs, (d–e) HRTEM images shows that nanotubes are integrated with bacteria proteins. (f) Schematic representative of interaction between CNTs and AMB1 surface proteins, MSP1 and flagellin. (g) The structural morphology of AMB1 bacteria (h) Raman spectra of CNTs and CNT-AMB1 structure.

Figure 3. Interactions between CNT and AMB-1 via surface protein, MSP1 and flagellin protein, flagellin: (a–b) All atom simulation trajectory screenshots for steered molecular dynamics and protein adsorption onto the DWNT; (c) Electrostatic energy between DWNT and the surface protein, MSP1 and flagellin domain D3 showing five times larger interaction for MSP1 compared to D3, (d) Van der Waals interactions between DWNT and the proteins MSP1 and D3 indicating a larger VDW interactions between DWNT and MSP1 compared to D3, (e) Root Mean Square Deviation (RMSD) showing the adsorption of the proteins at ~7 ns onto the DWNT surface, (f) Force vs Time plot showing the presence of repulsive forces between the DWNT and the proteins indicating the role of these proteins and hence AMB1 as a crosslinker molecule for 3D CNT scaffold.

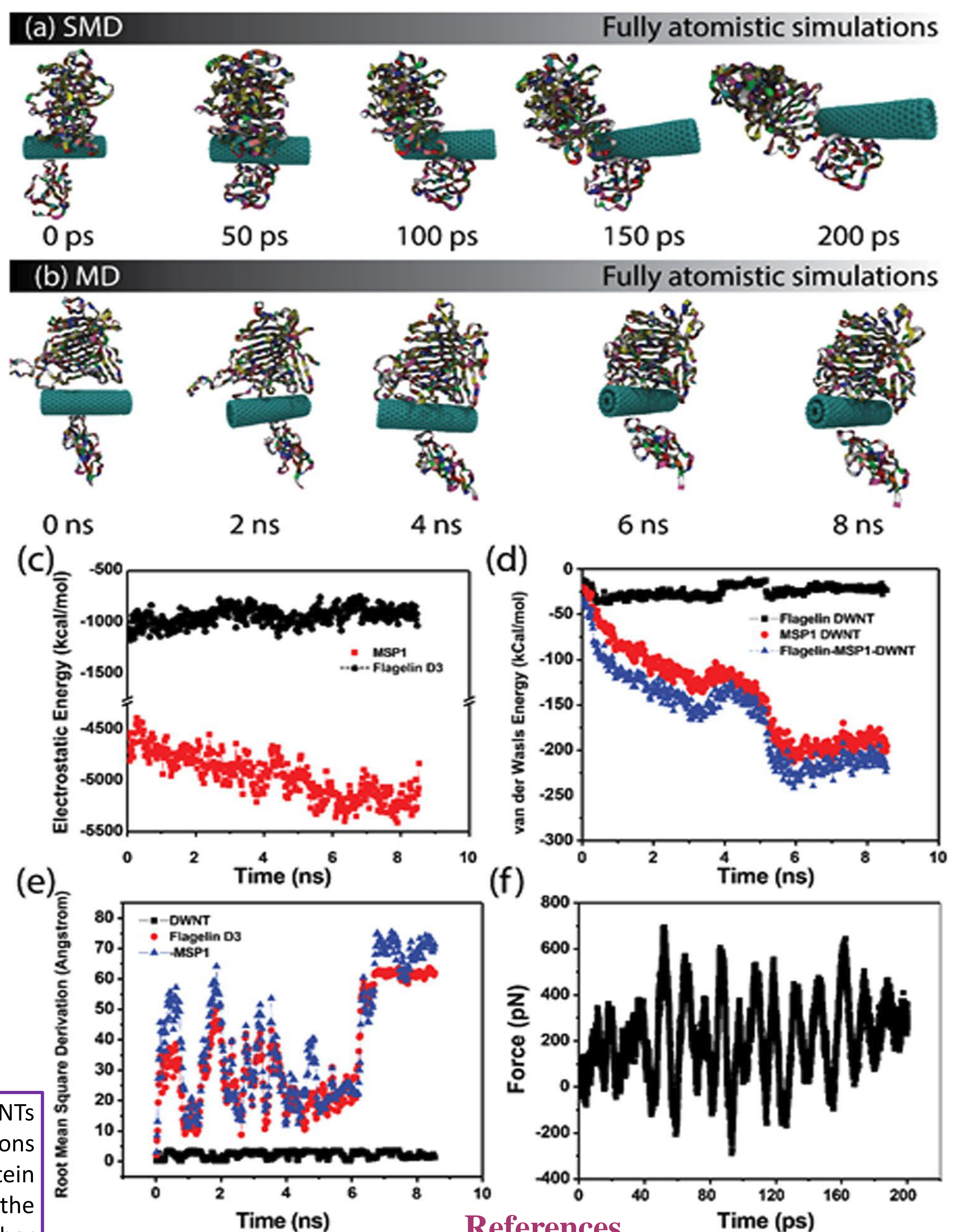
Materials and Methods

Experiments:

- Carbon nanotubes were obtained from *cheaptubes.com* (Outer Diameter: 20–30 nm, length 10–30 μm). *M. Magneticum* AMB-1 (The average size of bacteria: 5–8 μm in length, 500 nm diameter) was purchased from the *American Type Culture Collection* (ATCC 700264) and microaerobically cultured in *magnetic spirillum growth medium*.
- Before autoclaving, 280 ml of the media was divided into 20 test tubes (14 ml each) and 0.001 g of CNTs was added to each test tube. Once sterilization was done, 0.5 ml of AMB-1 (~106 cells per ml) culture was inoculated per test tube and incubated at 28 °C for one week.
- After one week, the *functionalized CNTs* were harvested by centrifuging the cultures at 7000 rpm for 30 minutes. The pellets were then allowed to dry overnight.
- For the electrode fabrication for *supercapacitor measurements*, CNT and CNT-bacteria (70 wt%) were further mixed with conducting carbon (20 wt%) and PVDF (10 wt%) as binder using N-methyl-2-pyrrolidone as solvent and 1M Na_2SO_4 as an electrolyte. The coin cell thus prepared was *tested by cyclic voltammetry measurement and galvanostatic charge discharge*.

MD and SMD (Steered Molecular Dynamics) Simulations:

- All-atom simulations (~100,000 atoms) using *VMD*³ and *NAMD*⁴ between MSP1, flagellin and DWNT (double walled carbon nanotube).
- Once the adsorption was achieved (~7ns), SMD⁵ was used in a constant velocity mode (0.25 $\text{\AA}/\text{ps}$, $k = 7 \text{ kcal/mol/\AA}^2$) for 200ps.
- CHARMM force field*⁶ and *TIP3*⁷ water model with neutralizing concentration of ions was used in accordance with the experimental procedure.
- Periodic boundary conditions* based on a *constant temperature* of 300K and a *constant pressure* of 1 Atm. were assumed.
- Data analysis* for the interactions taking place between the AMB-1 cell surface proteins and DWNT was performed using VMD & TCL.



References

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We report renewable and scalable light-weight 3D porous macrostructure using CNTs and *Magnetospirillum magneticum* (AMB-1) bacteria. To understand the interactions between CNTs and AMB-1 bacteria's cell surface protein MSP-1 and flagellin protein flagellin, SMD simulations were used, which are in good agreement with the experimental data. The 3D CNTs-AMB-1 nanocomposite scaffold is further demonstrated as an electrode for supercapacitor applications with the highest capacitance of 177.8 F/g, which improved more than six times compared to pure CNTs. We propose that magnetite and heteroatoms of the bacterial structure have an important role for the charging and discharging capacity of the 3D CNT-AMB-1 structure.